

**Product Name:** BAN ORL 24

**Catalog No.:** 3661

**Batch No.:** 3

CAS Number: 1401463-54-4

IUPAC Name: (2*R*)-1-(Phenylmethyl)-*N*-[3-(spiro[isobenzofuran-1(3*H*),4'-piperidin]-1-yl)propyl-2-pyrrolidinecarboxamide dihydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>27</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>·2HCl·½H<sub>2</sub>O

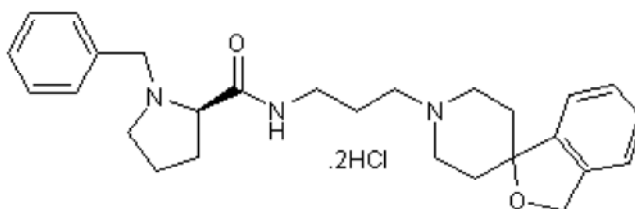
**Batch Molecular Weight:** 515.52

**Physical Appearance:** Off White solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.28 (Dichloromethane:Methanol [95:5])

**HPLC:** Shows >99.2% purity

**Chiral HPLC:** Shows >99.7% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +10.8 (Concentration = 1, Solvent = Water)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.91	7.43	8.15
Found	62.75	7.55	7.96

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Potent and selective NOP receptor antagonist (IC<sub>50</sub> values are 0.27, 2500, 6700 and > 10000 nM for NOP, κ-, μ- and δ-receptors respectively). Inhibits nociceptin-induced stimulation of [<sup>35</sup>S]-GTPγS binding and Ca<sup>2+</sup> mobilization in CHO cells in vitro and antagonizes NOP agonist-induced reduction in locomotor activity in vivo. Brain penetrant.

**Physical and Chemical Properties:**

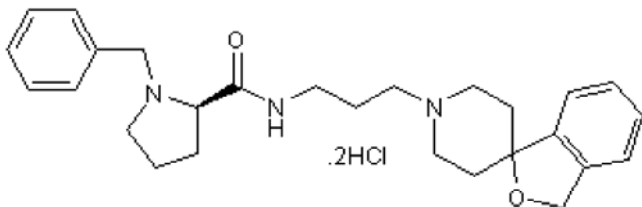
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Batch Molecular Weight: 515.52

Physical Appearance: Off White solid

**Minimum Purity:** ≥97%

**Batch Molecular Structure:**



**Storage:** Store at -20°C. This product is packaged under an inert atmosphere.

**Solubility & Usage Info:**

water to 100 mM

DMSO to 100 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Fischetti et al** (2009) Pharmacological characterization of the nociceptin/orphanin FQ receptor non peptide antagonist compound 24. *Eur.J.Pharmacol.* **614** 50. PMID: 19445927.

**Liao et al** (2009) 1-Benzyl-*N*-[spiroisobenzofuran-1(3*H*),4'-piperidin-1-yl]propyl]pyrrolidine-2-carboxamide (compound 24) antagonizes NOP receptor-mediated potassium channel activation in rat periaqueductal gray slices. *Eur.J.Pharmacol.* **606** 84. PMID: 19374842.

**Goto et al** (2006) Identification of a novel spiro piperidine opioid receptor-like 1 antagonist class by a focused library approach featuring 3D-pharmacophore similarity. *J.Med.Chem.* **49** 847. PMID: 16451050.

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